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CLASSICAL CALCULATION OF THE DIFFERENTIAL
CROSS SECTION FOR SCATTERING OF HYDROGEN
MOLECULAR IONS FROM HEAVY ATOMS

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CLASSICAL CALCULATION OF THE
DIFFERENTIAL CROSS SECTION FOR
SCATTERING OF HYDROGEN MOLECULAR
IONS FROM HEAVY ATOMS

by

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ABSTRACT

The primary problem in the calculation of the differential scattering cross section for hydrogen molecular ions is the derivation of an approximate expression for the probability that the hydrogen molecular ion will be oriented, prior to impact, in such a way as to avoid disruption during scattering. Using a simple model, an approximate expression for the orientation probability is obtained.

Differential cross sections for the scattering of hydrogen molecular ions from carbon and krypton are calculated using classical scattering theory and the derived orientation probability. Impact energies of 100 to 1000 electron volts are considered. In addition differential cross sections for protons scattered from carbon and krypton are presented.

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1. INTRODUCTION

Bates, Cook, and Smith, have presented a classical theory of ion-molecular rearrangement collisions at high impact energies^[1].

Using proton-methane collisions as an example a brief outline of the theory follows.

In Figure 1 m_1 is the impacting proton, m_2 is one of the hydrogen atoms of the methane molecule and M_k is the carbon atom of the methane molecule. In this collision $m_1 = m_2 \ll M_k$. For capture to occur $\vec{V}_1' \approx \vec{V}_2''$. From these two conditions and the conservation of linear momentum and energy it can be shown that $\theta_2'' \approx 90^\circ$ and $\theta_1 \approx 45^\circ$. Thus, for this case, capture of the hydrogen atom of the methane by the incident proton to form hydrogen molecular ions may occur at an angle of approximately 45° . Bates, Cook and Smith have calculated a cross section for the production of hydrogen molecular ions by this process^[1].

An experimental difficulty may arise in a measurement of the cross section for the production of H_2^+ by this double scattering process if the incident proton beam contains some significant number of H_2^+ . If the cross section for scattering of H_2^+ from the carbon atom is much larger than the cross section for H_2^+ production by capture, then a measurement of the production cross section would be impossible unless a pure source of protons were used. In order to determine the relative magnitudes of these two differential scattering cross sections a calculation of the differential cross section of H_2^+ ions scattered from heavy atoms is presented.

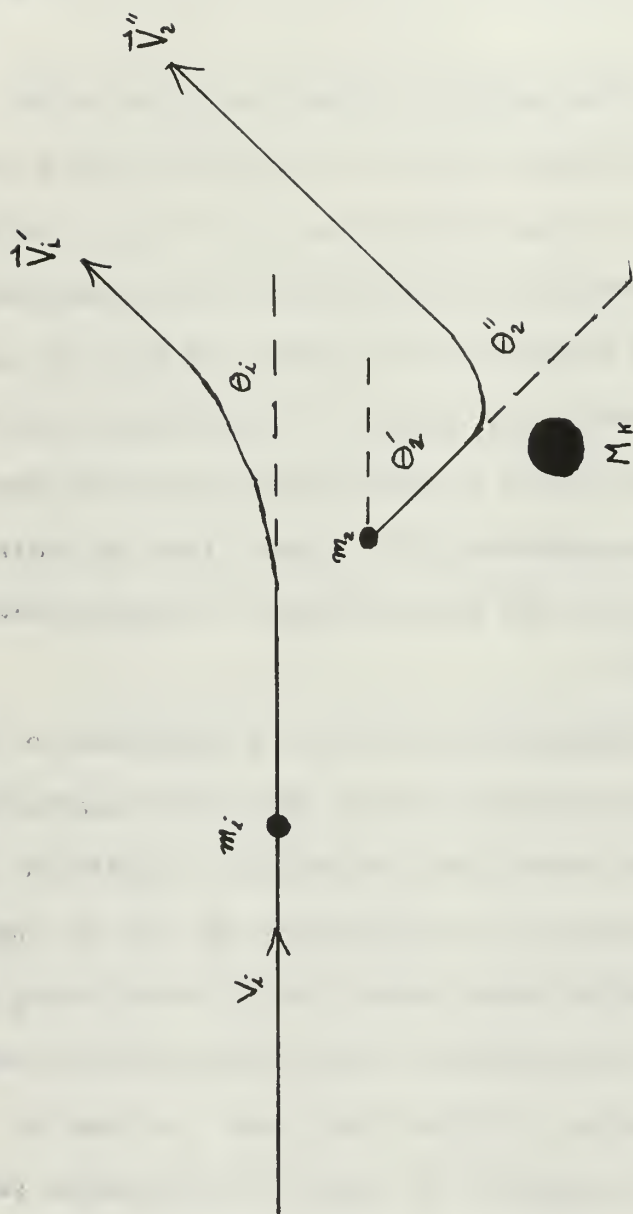


Figure 1. Schematic illustration of the capture process

2. THE MODEL

The hydrogen molecular ion is linear with an inter atomic spacing of approximately two angstroms. For randomly oriented impacting H_2^+ ions this implies a possible difference in impact parameter for the individual atoms of as much as two angstroms. If the difference in impact parameters is great enough, the velocities of the two atoms after scattering may differ by enough to cause their relative energy to exceed the binding energy of the molecule. The molecule will then be disrupted and can not be considered an H_2^+ scattering event.

Even at zero difference in impact parameter disruption of the molecule may occur because of the following consideration. In a spherically symmetric potential, such as that used in this calculation, each particle remains in a plane, defined by the scattering axis and a line from the scattering axis to the particle, during and following the collision. If the angle between the planes is great enough the difference in the velocities of the two atoms, after scattering, may be such that the molecule is disrupted.

Figure 2 shows the relationship between the scattering planes and the scattering axis. $\zeta\Phi$ is the angle between the scattering planes.

The condition that the molecule remains intact may be stated as $D > \frac{1}{2} \mu (\zeta V)^2$ where D is the binding energy, ζV is the relative velocity of the two particles and $\frac{1}{2} \mu (\zeta V)^2$ gives the relative energy of the two particles. Using the symbol ΔV for the maximum allowable ζV the limiting condition for nondisruption becomes:

$$D = \frac{1}{2} \mu (\Delta V)^2 .$$

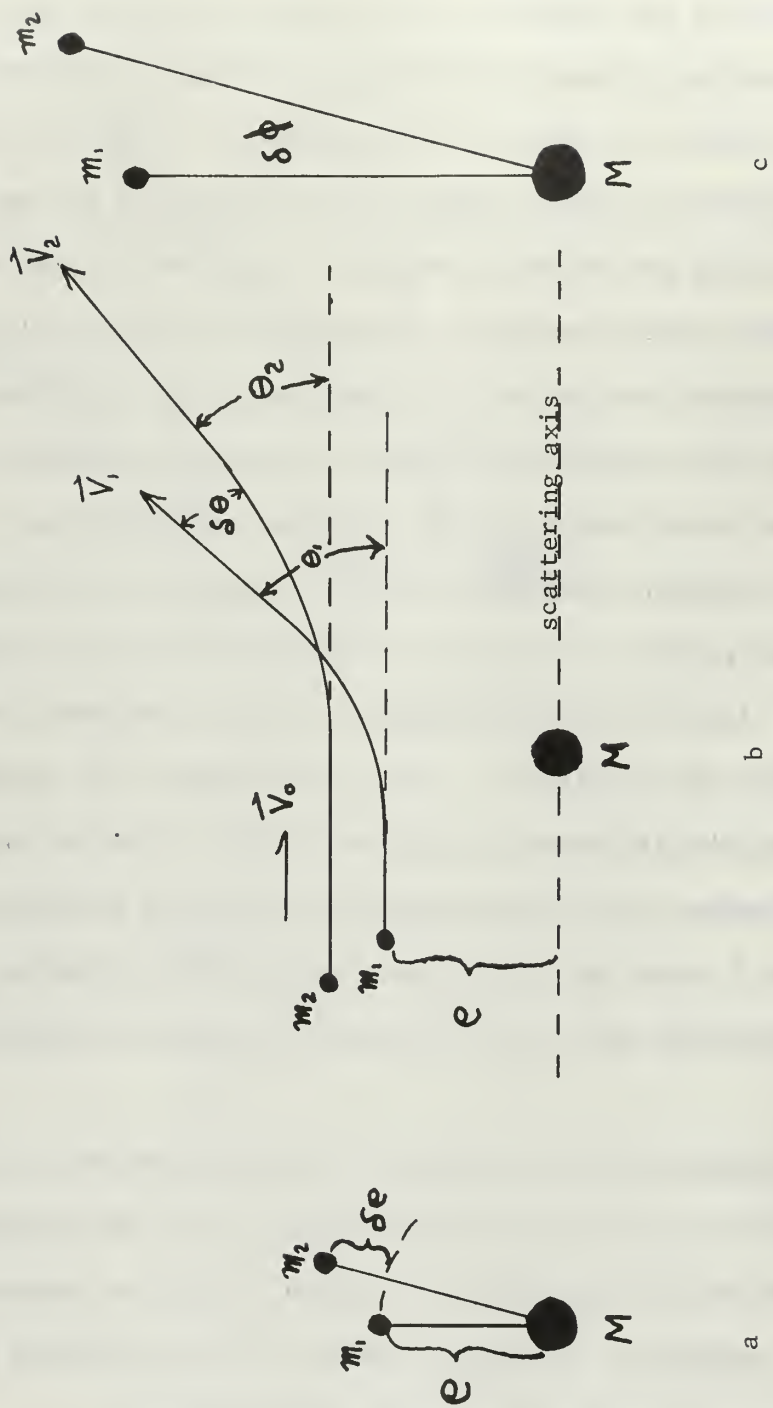


Figure 2. Illustration of scattering model.

Thus both the difference in impact parameter $\zeta\rho$ and the angle between the scattering planes must be such that the above condition is satisfied. This limitation on the orientation of the impacting molecule leads to an orientation probability that must be considered in the calculation of the differential scattering cross section for hydrogen molecular ions.

For high impact energies and small impact parameters each atom of the H_2^+ may be treated as a proton. That is, the effective charge may be taken as one for each particle. The calculation of the differential cross section for H_2^+ ions may then be approached in the following way. For a given energy and impact parameter calculate the scattering angle, and the differential cross section for that angle, for one proton whose velocity is V_0 , the velocity of the H_2^+ . Then determine the probability that the "second" particle is oriented with respect to the "first" particle in such a way that its scattering angle is within $\Delta\theta$ of θ and its scattering plane makes an angle of less than $\Delta\Phi$ with the scattering plane of the first particle. The differential cross-section for H_2^+ scattering will then be given by: $\sigma_{H_2^+}(\theta) = \sigma_{H^+}(\theta) P$, where P is the orientation probability. This is then done over a range of impact parameters and for several energies.

3. CALCULATION of $\sigma_{H^+}(\theta)$

The calculation of $\sigma_{H^+}(\theta)$ for the "first" particle was done using the method suggested by Bates, Cook and Smith^[1]. The potential used for the calculation was a shielded potential of the form,

$$V(R) = \frac{Ze^2}{R} (Me^{-mR} + Ne^{-nR} + Le^{-lR}) \text{ due to Byatt}^{[2]}. \text{ Calculations were made}$$

for both carbon and krypton. Byatt lists several potentials in reference 2, all of which may be conveniently used in the computer

program in appendix 2. The cross section was calculated for impact parameters from 0 - 5 a_0 in increments of 0.05 a_0 (a_0 is the radius of the Bohr orbit) and for energies from 100ev to 1000ev in steps of 100ev. The details of the calculation are shown in appendix 1.

4. CALCULATION OF THE ORIENTATION PROBABILITY.

The condition $\Delta V = \left(\frac{4D}{M_H}\right)^{\frac{1}{2}}$ may, for convenience, be put in terms of the energy of the H_2^+ . $E_{H_2^+} = \frac{1}{2}(2M_H)V_0^2 = M_H V_0^2$ or $M_H = \frac{E_{H_2^+}}{V_0^2}$ then $\Delta V = \left(\frac{4D}{E_{H_2^+}}\right)^{\frac{1}{2}} V_0$. This limiting condition implies a relationship

between $\zeta\theta$ and $\zeta\Phi$ such that $\Delta V = F(\zeta\theta, \zeta\Phi)$. $\zeta\theta$ is related to $\zeta\rho$ by $\zeta\theta = \rho\zeta\rho/\sigma_H(\theta) \sin\theta$ in the center of mass coordinate system.

Therefore $\Delta V = G(\zeta\Phi, \zeta\rho)$ gives a relationship between $\zeta\Phi$ and $\zeta\rho$. Since ΔV is a constant for a given energy and impact parameter, there exists some relationship between $\zeta\rho$ and $\zeta\Phi$ such that $\zeta\Phi = f(\zeta\rho)$. $\zeta\Phi = f(\zeta\rho)$ defines a curve in a plane perpendicular to the scattering axis. The second particle must pass through the area on the plane bounded by this curve if disruption is to be avoided.

The randomly oriented H_2^+ can be considered as defining a sphere the center of which is the "first" atom and whose radius is ℓ , the inter atomic spacing.

In Figure 3, A is the area on the surface of the hemisphere contained within the surface defined by $\zeta\rho = f(\zeta\Phi)$. The ratio of this area to the area of a hemisphere of radius ℓ gives the fraction of the H_2^+ ions which are oriented in such a way as to avoid disruptions. Thus the orientation probability, P is given by: $P = A/2\pi\ell^2$. No exact solution has been obtained for the orientation probability.

As an approximation to the orientation probability the following simplifications were made.

Assuming the target atom to be infinitely massive, there will be no change in the magnitude of the velocity of either atom of the hydrogen molecular ion. Since they then have the same initial speed V_0 , $V_1 = V_2 = V_0$. When $\zeta\Phi = 0$ the particles are scattered in the same plane as shown in Figure 4a. Then, assuming $\Delta\theta$ is small

$$\Delta V \approx V_0 \Delta\theta \text{ or } \Delta\theta \approx \left(\frac{4D}{E_{H_2^+}} \right)^{\frac{1}{2}}. \text{ When } \zeta\theta = 0 \text{ (which implies } \zeta\rho = 0)$$

the relationship between the individual atoms is as shown in Figure 4b.

Then $\Delta V \approx (V_0 \sin\theta) \Delta\Phi \approx \left(\frac{4D}{E_{H_2^+}} \right)^{\frac{1}{2}} V_0$ or $\Delta\Phi = \left(\frac{4D}{E_{H_2^+}} \right)^{\frac{1}{2}} \left(\frac{1}{\sin\theta} \right)$ these approximations then give independent maxima for $\zeta\Phi$ and $\zeta\theta$. $\Delta\theta$ is related to $\Delta\rho$ by Δ

$$\Delta\rho = \frac{\sigma_{H^+}(\theta) \sin\theta \Delta\theta}{\rho} \text{ or } \Delta\rho = \frac{\sigma_{H^+}(\theta) \sin\theta \left(\frac{4D}{E_{H_2^+}} \right)^{\frac{1}{2}}}{\rho}$$

The above restriction on $\Delta\rho$ implies that the second particle must be contained between two coaxial cylinders whose axis is the scattering axis and whose radii are $\rho - \Delta\rho$ and $\rho + \Delta\rho$ respectively. The condition

$$\Delta\Phi \approx \left(\frac{4D}{E_{H_2^+}} \right)^{\frac{1}{2}} \left(\frac{1}{\sin\theta} \right)$$

puts a limit on the angular separation of the scattering planes. The limits on $\Delta\Phi$ and $\Delta\rho$ then confine the second particle to lie on the surface of a hemisphere of radius ℓ contained between the two scattering planes and the two cylindrical surfaces. Figure 5 illustrates.

This area, on the surface of the hemisphere, divided by the area of the hemisphere then gives an approximation to the orientation probability.

As a further approximation, this area was assumed small and taken to be the plane area given by $A \approx \rho(2\Delta\Phi) (2\Delta\rho)$; which then gives, as an estimate of the orientation probability, $P \approx \frac{2\rho\Delta\Phi\Delta\rho}{\pi\ell}$.

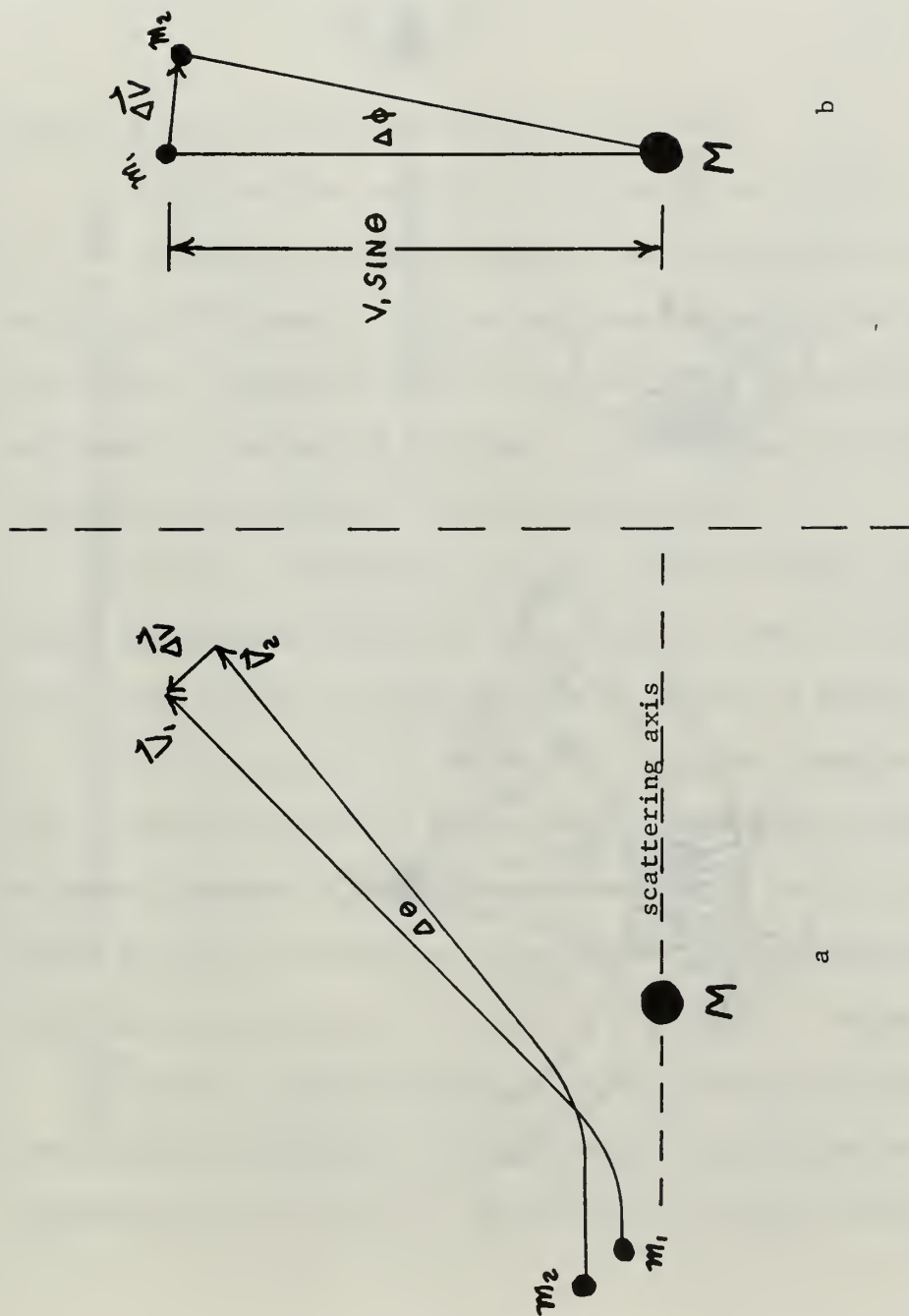


Figure 4. Illustration of the approximation to the orientation probability

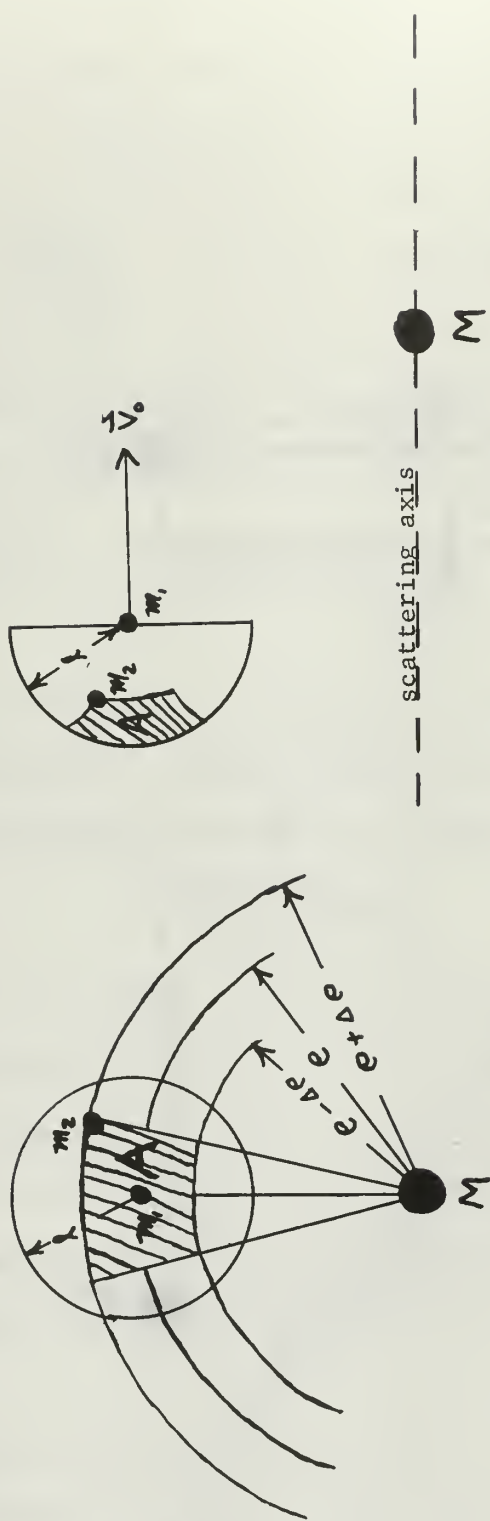


Figure 5. Illustration of the approximate probability area

5. RESULTS AND DISCUSSION

Everhart, et al, have calculated the differential cross section for scattering from a screened Coulomb potential^[3]. The results are presented in terms of a , the screening length, given by:

$$a = \left[\frac{a_0}{Z_1^{3/2} + Z_2^{3/2}} \right]^{1/2}$$

and b , the collision diameter, given by:

$$b = \frac{Z_1 Z_2 e^2}{\frac{1}{2} \mu V^2}$$

where μ = the reduced mass of the system.

V = the relative velocity of projectile and target.

As a check on the calculation of the cross section for proton scattering the computer program used for the calculation was run using the screened Coulomb potential of carbon and a proton impact energy such that the ration b/a was equal to 1. The results of this calculation were within 2.34% of those of Everhart et al.

The actual calculations were made using the Byatt potentials of carbon and krypton with proton impact energys from 50 to 500 electron volts. The results are presented in the graphs of Figures 6 and 7.

The cross section for the scattering of the hydrogen molecular ion for impact energies of 100 to 1000 electrons volts (corresponding to proton energies of 50 to 500 electron volts) then is the cross section for proton scattering multiplied by the orientation probability. These cross sections are presented in the graphs of Figures 8 and 9.

Under the assumption that the speeds of the two particles are the same following scattering, the $\Delta\theta$ used in the orientation probability approximation is due only to the difference in the directions of the

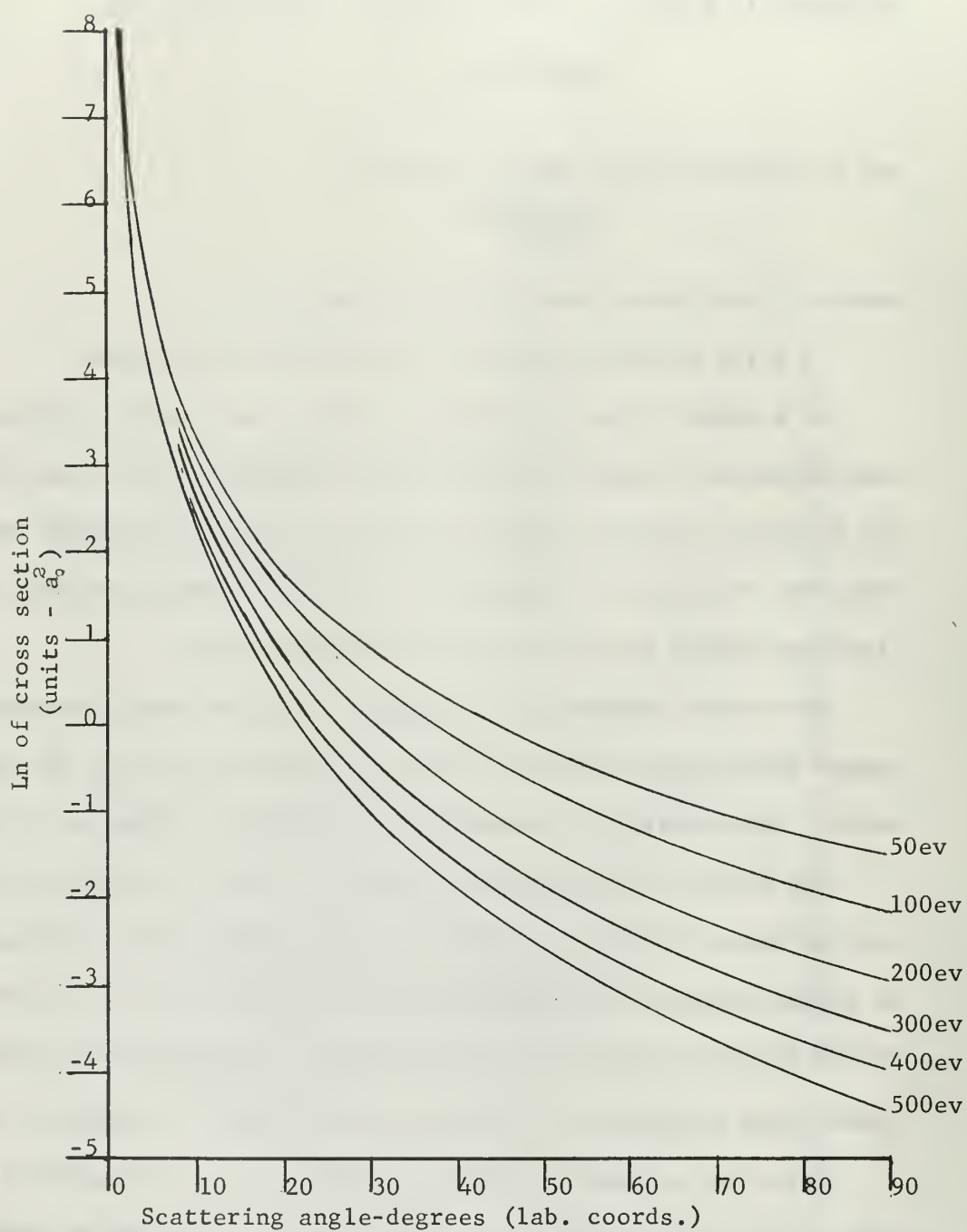


Figure 6. Graph of the logarithm of the differential scattering cross section versus scattering angle for protons on carbon.

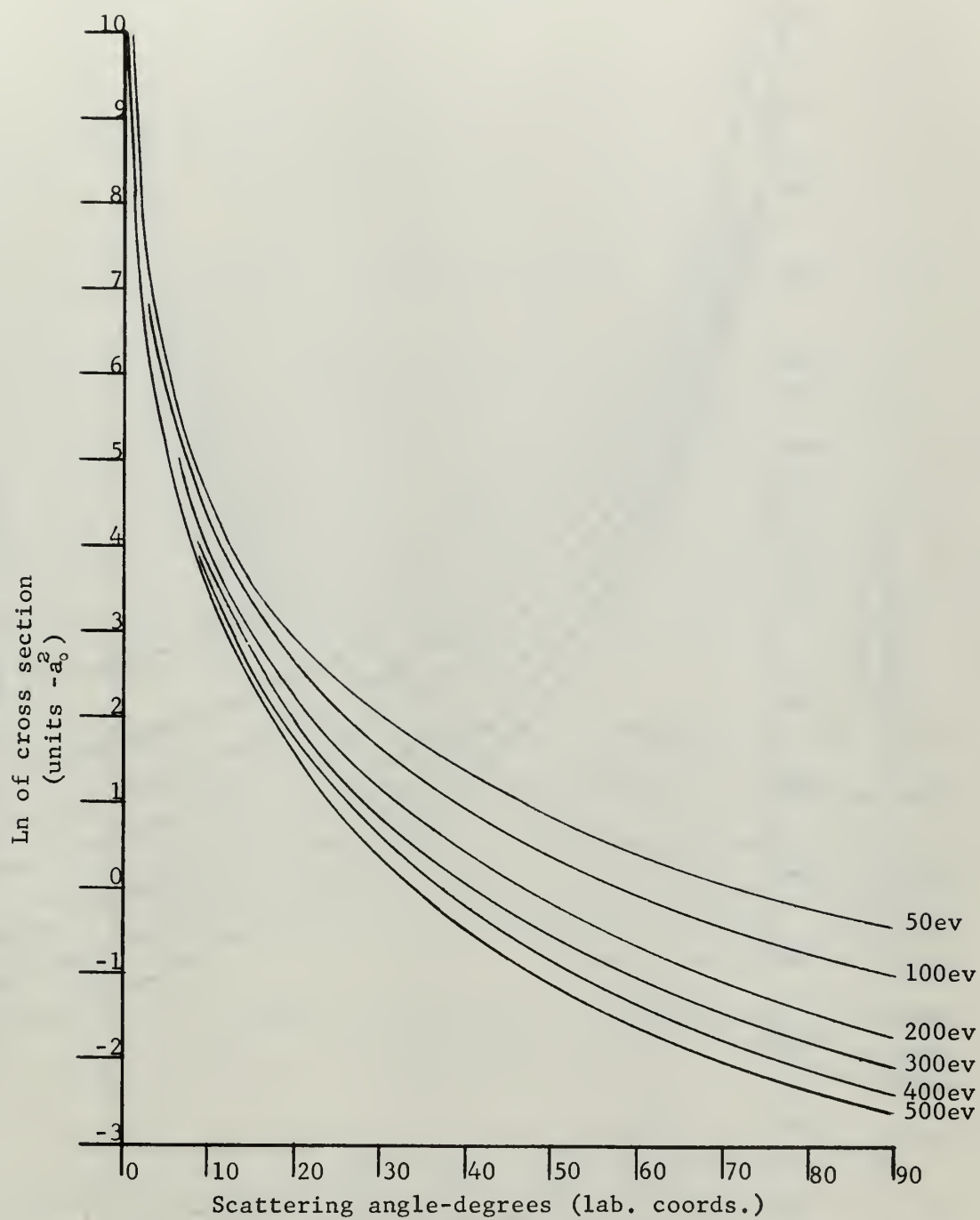


Figure 7. Graph of the logarithm of the differential scattering cross section versus scattering angle for protons on krypton.

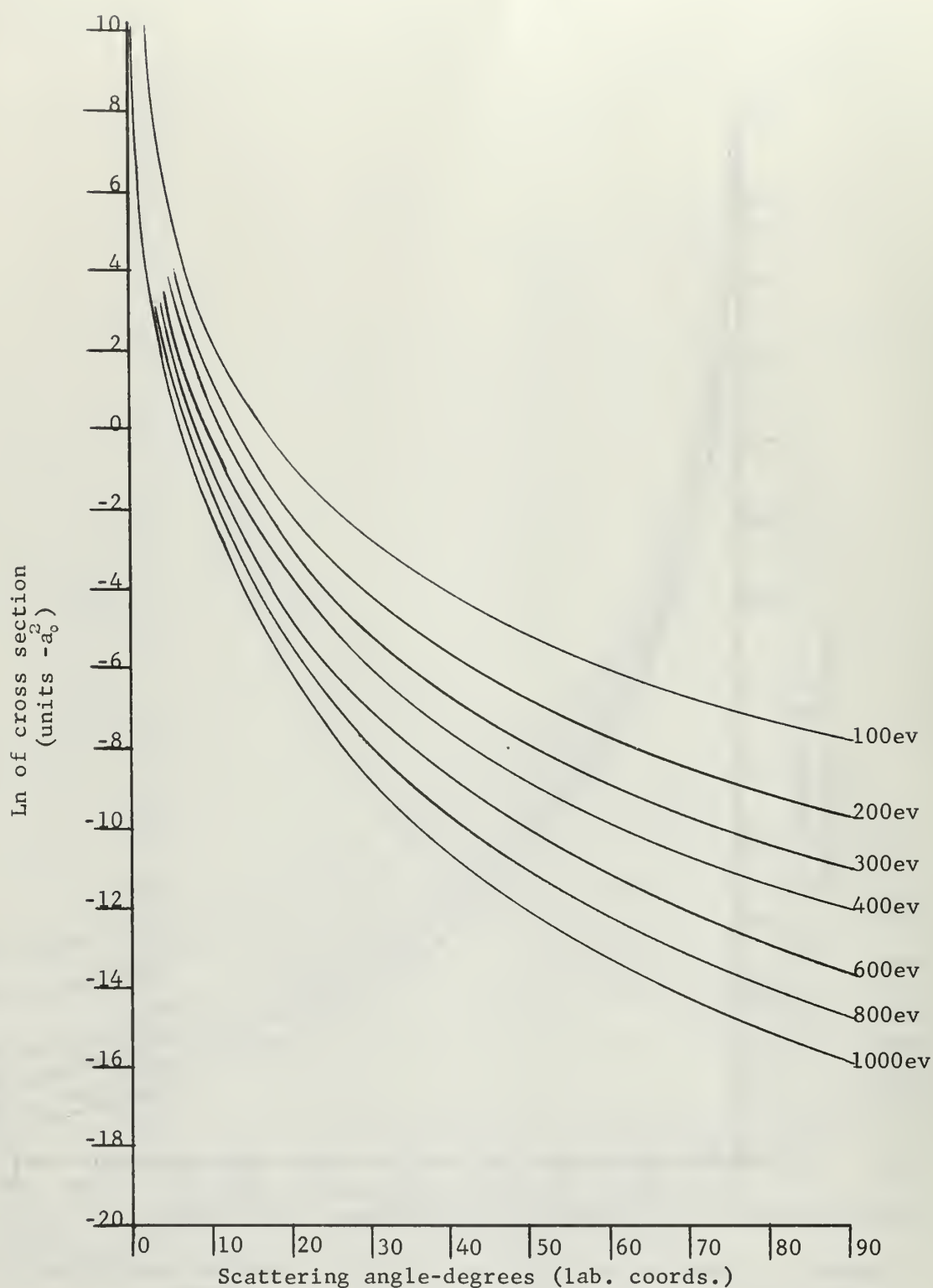


Figure 8. Graph of the logarithm of the differential scattering cross section versus scattering angle for hydrogen molecular ions on carbon.

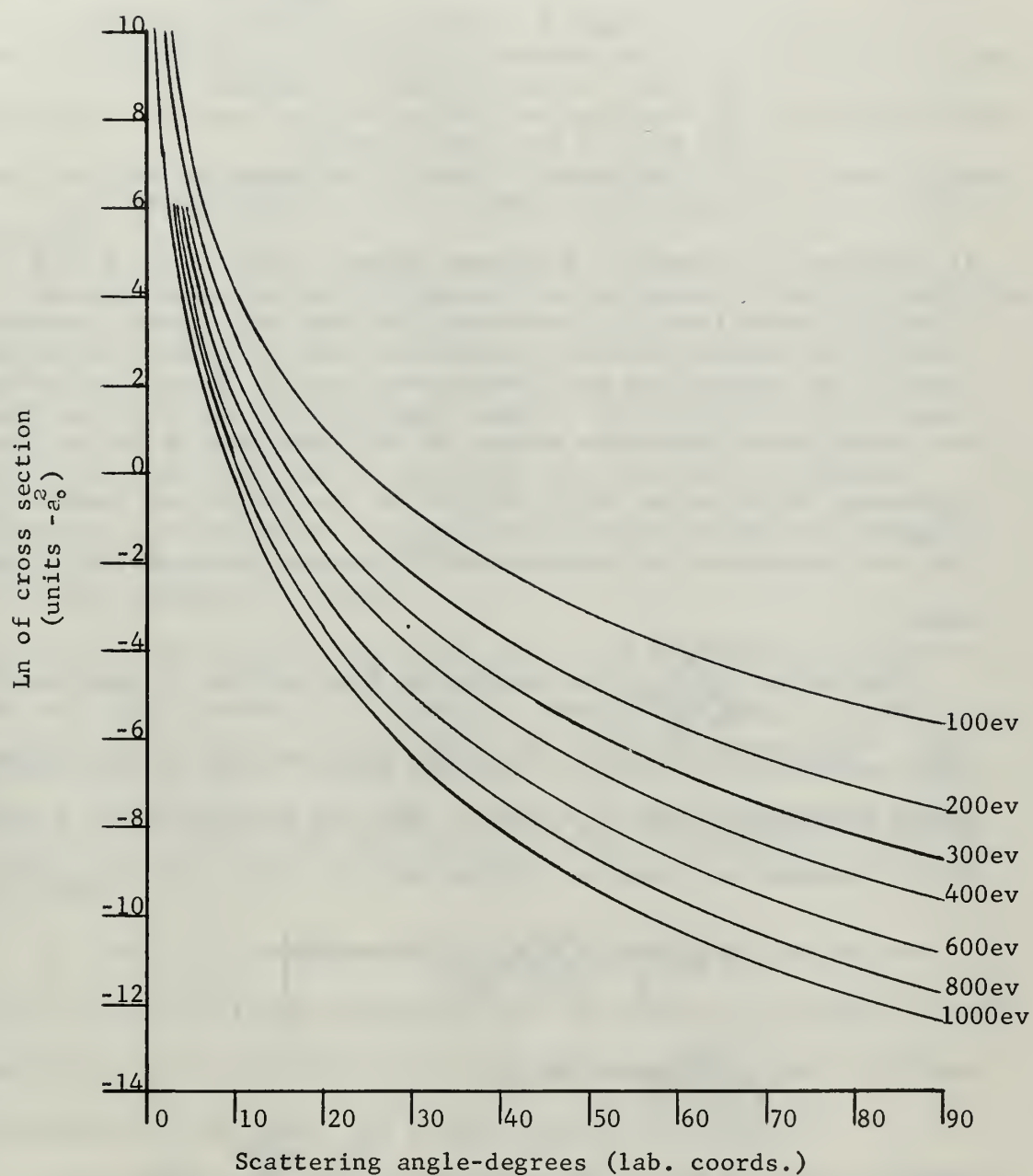


Figure 9. Graph of the logarithm of the differential scattering cross section versus scattering angle for hydrogen molecular ions on krypton.

velocity vectors. The speed of a particle scattered through an angle θ is given by:

$$V = V_0 \left[1 - \frac{2M_t M_H}{(M_H + M_t)^2} (1 - \cos\theta) \right]^{\frac{1}{2}}$$

where V = the speed of a projectile particle scattered through an angle θ in the C.M. Coordinate system,

M_H = Mass of the projectile particle,

M_t = Mass of the target particle

and V_0 = initial speed of the projectile particle.

If the speeds of particles scattered through angles θ and $\theta + \zeta\theta$ differ by enough that ζV_s , resulting from this difference, is greater than ΔV , the maximum for non disruption, then the H_2^+ will be disrupted due to the speed difference alone. If $\Delta\theta_s \gg \Delta\theta$, then $\Delta\theta$ (due to the difference in direction only) will be the more stringent condition and the error introduced by ignoring the difference in speeds may be assumed small.

The factor $\frac{2M_t M_H}{(M_H + M_t)^2}$, for scattering from carbon, is approximately $\frac{24}{169}$. The factor $(1 - \cos\theta)$ is always less than one for scattering angles between zero and 90 degrees. Thus the expression for V above can be expanded in a series. Taking only the first two terms gives,

$$V = V_0 \left[1 - \frac{M_t M_H}{(M_t + M_H)^2} (1 - \cos\theta) \right]$$

$$\text{then } \zeta V = -V_0 \frac{M_t M_H}{(M_t + M_H)^2} \sin\theta \zeta\theta$$

$$\text{when } \zeta V_s = \Delta V \text{ and } \zeta\theta_s = \Delta\theta_s, \text{ then } |\Delta\theta_s| = \frac{(M_t + M_H)^2}{M_t M_H \sin\theta} \left(\frac{\Delta V}{V_0} \right)$$

but $\Delta V = \left(\frac{4D}{M_H} \right)^{\frac{1}{2}}$ and $V_o = \left(\frac{E_{H_2^+}}{M_H} \right)^{\frac{1}{2}}$

Therefore $\frac{\Delta V}{V_o} = \left(\frac{4D}{E_{H_2^+}} \right)^{\frac{1}{2}}$, which is just the $\Delta\theta$ due to the difference in direction of the velocity vectors.

Therefore $\Delta\theta = \frac{(M_H + M_t)^2}{M_H M_t \sin\theta}$. For carbon, then $\Delta\theta_s \geq 14 \Delta\theta$.

This implies that the H_2^+ will be disrupted due to the difference in the directions of the velocities of the two particles at a $\Delta\theta$ which is much less than the $\Delta\theta_s$ required to cause a disruption due to a speed difference only.

Because there is some difference in the speeds of the two particles the relative energy of the particles is somewhat greater than that predicted with the speeds assumed equal. Thus disruption will occur more often than predicted by the model used for the calculation. Therefore, the assumption of equal speeds tends to make the probability factor somewhat too large.

The use of separate maxima for $\Delta\phi$ and $\Delta\Phi$ introduces an error in that the final probability expression contains the product of the maximum values, each of which was derived under the assumption that the other was zero. This error tends to make the probability factor too large.

In view of the small values of P, (representative values are listed in Table 1.) the assumption that the area on the surface of the hemisphere can be approximated by a plane area would seem to be reasonable for, at least, the higher angles and energies.

The conclusion is that the probability factor is in general somewhat too large thus causing the calculated cross sections for

Energy (in ev)	θ (Lab.)	Carbon	θ (Lab.)	Krypton
		P		P
100	83.65	1.95×10^{-3}	87.88	5.08×10^{-3}
100	45.62	7.72×10^{-3}	45.23	2.22×10^{-2}
100	10.68	2.10×10^{-1}	10.32	6.38×10^{-1}
500	88.88	9.18×10^{-5}	83.45	2.68×10^{-4}
500	42.35	7.08×10^{-4}	45.39	1.66×10^{-3}
500	10.37	2.30×10^{-2}	10.10	7.00×10^{-2}
1000	75.20	1.72×10^{-5}	86.47	6.04×10^{-5}
1000	47.62	7.12×10^{-5}	46.80	3.12×10^{-4}
1000	10.35	7.46×10^{-3}	10.13	2.32×10^{-2}

Table 1. Representative values of the orientation probability.

hydrogen molecular ion scattering to be too large.

In Figure 10 the curve marked $\sigma_{H_2^+}(45^\circ)$ is the differential scattering cross section for H_2^+ from carbon at a scattering angle of 45° as a result of this calculation. The impact energies plotted are from 100ev to 1000ev. The curve labeled $\sigma(H_2^+ + CH_4 \longrightarrow CH_3 + H_2^+)$ is the cross section for the capture of a hydrogen atom from the methane molecule by an impacting proton. This curve is a result of calculations based on the reaction cross section as derived by Bates, Cook and Smith^[1]. Figure 10 shows the cross section for scattering of H_2^+ from carbon at 45° to be somewhat more than an order of magnitude greater than the cross section for the reaction $H^+ + CH_4 \longrightarrow CH_3 + H_2^+$. As a result, in order to measure the reaction cross section it would appear that a proton beam free of H_2^+ will be necessary.

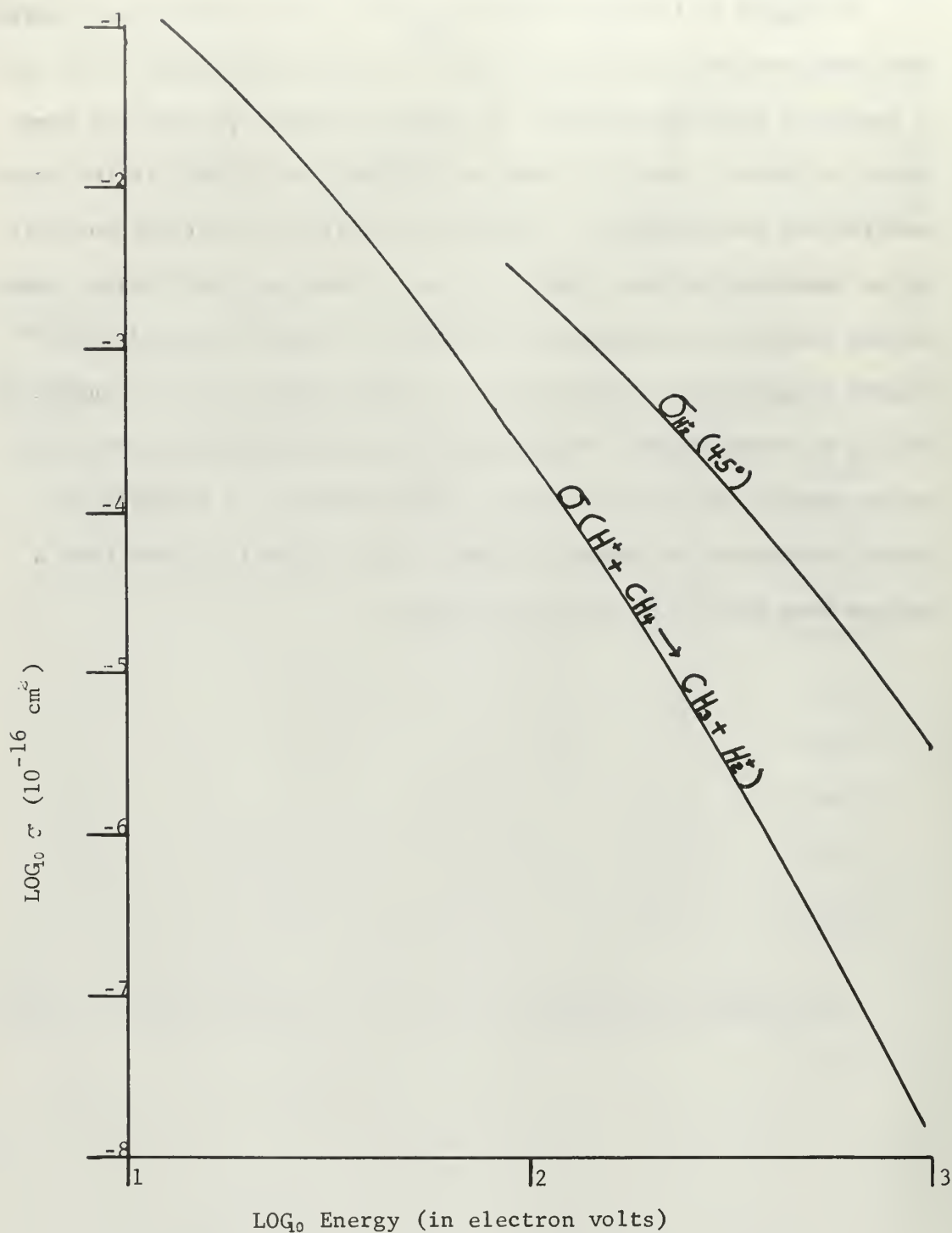


Figure 10. Comparison of reaction and scattering cross sections.

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APPENDIX 1

CALCULATION OF $\sigma_{H^+}(\theta)$

The classical differential scattering cross section in the center of mass coordinate system is given by:

$$\sigma(\theta) = e \left[\sin \theta \left| \frac{d\theta}{de} \right| \right]^{-1} \quad (1)$$

where e is the impact parameter and θ is the scattering angle in the

center of mass coordinate system. θ is related to e by: $\theta = \pi - 2eU$ (2)

where

$$U = \int_{r_0}^{\infty} \frac{dr}{r^2 \left[1 - \frac{V(r)}{\frac{1}{2}\mu V_0^2} - \frac{e^2}{r^2} \right]^{1/2}} \quad (3)$$

in which r_0 is the largest positive root of

$$1 - \frac{V(r)}{\frac{1}{2}\mu V_0^2} - \frac{e^2}{r^2} = 0 \quad (4)$$

and μ = the reduced mass of the system

$V(r)$ = the scattering potential.

V_0 = the velocity of the impacting particle in the lab

coordinate system when the target particles are considered

to be at rest.

The potential as given by Byatt,^[2] is

$$V(r) = \frac{z_1 z_2 e^2}{r} (D e^{\alpha r} + E e^{\beta r} + F e^{\gamma r}) \quad (5)$$

after converting $V(r)$ to electron volts and letting $r = R a_0$, there results:

$$V(R) = \frac{1}{R} (A e^{\alpha R} + B e^{\beta R} + C e^{\gamma R}) \quad (6)$$

Where

	For Carbon	For Krypton
A=	204.136	328.635
B=	-71.856	588.600
C=	31.029	63.765
α =	-1.700	-1.086
β =	-2.895	-4.961
γ =	-8.808	-26.110

The quantity $\frac{1}{2}\mu V_0^2$ can be put in terms of the energy of the H_2^+ in electron volts in the lab. coordinate system.

$$V_0^2 = \frac{2 E_{H_2^+}}{M_{H_2^+}} = \frac{2 E_{H_2^+}}{2 M_H} = \frac{E_{H_2^+}}{M_H}$$

$\mu = \frac{M_H M_T}{M_H + M_T}$ in which the mass, M_T , is the mass of the target atom.

Define $ET = \frac{1}{2} \left(\frac{M_H M_T}{M_H + M_T} \right) \frac{E_H}{M_H}$ (7)

Define $V = \frac{V(R)R}{ET}$ (8)

Then R_0 is the root of

$$1 - \frac{V}{R} - \frac{e^2}{R^2} = 0 \quad (9)$$

The root of this equation was found using the Newton-Raphson method

which is $R_{n+1} = R_n - \frac{f(R_n)}{f'(R_n)}$ (10)

where $f(R) = 1 - \frac{V}{R} - \frac{e^2}{R^2}$ (11)

and $f'(R) = \frac{V - R DV}{R^2} + \frac{2e^2}{R^3}$ (12)

in which DV is defined by

$$DV = \frac{dV}{dR} = \frac{(A\alpha e^{\alpha R} + B\beta e^{\beta R} + C\gamma e^{\gamma R})}{ET} \quad (13)$$

then

$$R_{n+1} = R_n - \frac{(R_n^2 - V R_n - e^2)}{(V - R_n DV + 2e^2/R_n)} \quad (14)$$

The integral, U, was evaluated using the Gauss-Mahler Quadrature formula as employed by Bates, Cook and Smith^[1]. The result is

$$U = \frac{\pi}{6R_0} \left[(\cos \frac{\pi}{12}) g(\cos \frac{\pi}{12}) + (\cos \frac{\pi}{4}) g(\cos \frac{\pi}{4}) + (\cos \frac{\pi}{6}) g(\cos \frac{\pi}{6}) \right] \quad (15)$$

where

$$g(x_i) = \left[1 - \frac{V(R_0/x_i)}{\frac{1}{2}\mu V_0^2} - \frac{e^2 x_i^2}{R_0^2} \right]^{-1/2} \quad (16)$$

in which the

$$x_i = \cos \frac{\pi}{12}, \cos \frac{\pi}{4} \text{ and } \cos \frac{\pi}{6} \quad (17)$$

To calculate $\left| \frac{d\theta}{de} \right|$ differentiate equation 2 with respect to e

$$\left| \frac{d\theta}{de} \right| = \left| 2e \frac{dU}{de} + 2U \right| \quad (18)$$

where

$$\frac{dU}{d\epsilon} = \frac{\partial U}{\partial \epsilon} + \frac{\partial U}{\partial R_0} \frac{dR_0}{d\epsilon} \quad (19)$$

$$\frac{\partial U}{\partial \epsilon} = \frac{\pi}{6R_0} \left[\left(\cos \frac{5\pi}{12} \right) \frac{\partial g(\cos \frac{\pi}{12})}{\partial \epsilon} + \left(\cos \frac{\pi}{4} \right) \frac{\partial g(\cos \frac{\pi}{4})}{\partial \epsilon} + \left(\cos \frac{\pi}{12} \right) \frac{\partial g(\cos \frac{5\pi}{12})}{\partial \epsilon} \right] \quad (20)$$

in which

$$\frac{\partial g(x_i)}{\partial \epsilon} = R_0 \epsilon x_i^2 \left[R^2 - VA - \epsilon^2 x_i^2 \right]^{-\frac{3}{2}} \quad (21)$$

and the X_i are as defined previously.

$\frac{dR_0}{d\epsilon}$ is obtained by differentiating

$$1 - \frac{V}{R_0} - \frac{\epsilon^2}{R_0^2} = 0$$

the result is

$$\frac{dR_0}{d\epsilon} = \frac{2\epsilon}{2\epsilon^2/R_0 - R_0 DV + V} \quad (22)$$

$$\frac{\partial U}{\partial R_0} = \frac{\pi}{6R_0} \left[\left(\cos \frac{5\pi}{12} \right) \frac{\partial g(\cos \frac{\pi}{12})}{\partial R_0} + \left(\cos \frac{\pi}{4} \right) \frac{\partial g(\cos \frac{\pi}{4})}{\partial R_0} + \left(\cos \frac{\pi}{12} \right) \frac{\partial g(\cos \frac{5\pi}{12})}{\partial R_0} \right] - \frac{U}{R_0} \quad (23)$$

in which

$$\frac{\partial g(x_i)}{\partial R_0} = \frac{R_0^3}{2} \left[R_0^2 - V R_0 x_i - \epsilon^2 x_i^2 \right]^{-\frac{3}{2}} \left[\frac{DV}{R_0} - \frac{V x_i}{R_0^2} - \frac{2\epsilon^2 x_i^2}{R_0^3} \right] \quad (24)$$

where the X_i are as defined previously,

APPENDIX 2

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	PRINT10	5
	10 FORMAT(1H1)	6
	PRINT54	7
	54 FORMAT(1H0,6HENERGY,9X,3HRHO,9X,4HR(0),3X,5HTHETA,7X,5HSIGMA,5X,	8
	112HORIENT,PROB.,1X,13HCROSS SECTION,5X,7HDELTA V//)	9
	DIMENSION EV(10),RHO(101),THETA(101),CSL(101),DEG(101),	10
	1THETAL(101),RATIO(10)	11
	DIMENSION X(900),Y(900),ITITLE(12),LABEL(12)	12
	DO 67 I=1,12	13
	67 ITITLE(I)=8H	14
	ITITLE(1)=8HJOB0634	15
	ITITLE(2)=8HFE1ST PL	16
	ITITLE(3)=8HOT OF LN	17
	ITITLE(4)=8HCS VS TH	18
	ITITLE(5)=8HETA FOR	19
	ITITLE(6)=8HHYDROGEN	20
	ITITLE(7)=8H MOLECUL	21
	ITITLE(8)=8HAR IONS	22
	ITITLE(9)=8HON CARBO	23
	ITITLE(10)=8HN IN LAB	24
	ITITLE(11)=8H COORD S	25
	ITITLE(12)=8HYSTEM	26
	GONTINUE	27
	A=204.136	28
	B=-71.856	29
	C=31.029	
	ALPHA=-1.700	
	BETA=-2.895	
	GAM=-8.808	

```

30 ITN=0
31 RHO(0)=-0.05
32 THETA(0)=0.
33 EV(0)=1100.
34 NO=1
35 DO 15 K=1,10
36 L=K-1
37 EV(K)=EV(L)-100.
38 R=200./EV(K)
39 NO=NO+1
40 IF(NO-2)19,16,17
41 16 NOA=1
42 GO TO 19
43 17 NOA=2
44 IF(NO-11)19,18,19
45 18 NOA=3
46 19 CONTINUE
47 LABEL(K)=4H 100
48 LABEL(1)=4H 100
49 LABEL(2)=4H 200
50 LABEL(3)=4H 300
51 LABEL(4)=4H 400
52 LABEL(5)=4H 500
53 LABEL(6)=4H 600
54 LABEL(7)=4H 700
55 LABEL(8)=4H 800
56 LABEL(9)=4H 900
57 LABEL(10)=4H1000
58 DO 6 J=1,101
59 N=J 1
60 RHO(J)=RHO(N)+0.05
61 1 X=EXPF(ALPHA*R)
62 Y=EXPF(BETA*R)
63 Z=EXPF(GAM*R)
64 XMP=1.008
65 XMT=12.011

```

```

66 ET=(0.5*(XMP*XMT)/(XMP+XMT))*EV(K)/XMP
67 V=(A*X+B*Y+C*Z)/ET
68 G=R**2-V*R-RHO(J)**2
69 DV=(A*ALPHA*X+B*BETA*Y+C*GAM*Z)/ET
70 H=V R*DV+2.*RHO(J)**2./R
71 RNEW=R-G/H
72 DIFR=ABSF((R-RNEW)/RNEW)
73 IF(DIFR-0.0001)4,2,2
74 2 ITN=ITN+1
75 IF(ITN-10000)3,7,7
76 3 R=RNEW
77 GO TO 1
78 4 CONTINUE
79 R=RNEW
80 V=(A*X+B*Y+C*Z)/ET
81 DV=(A*ALPHA*X+B*BETA*Y+C*GAM*Z)/ET
82 IF(R-RHO(J))7,120,61
83 61 QI=COSE(3.14159/12.)
84 SJ=COSE(3.14159/4.)
85 TK=COSE(3.14159*5./12.)
86 QIA=EXP(ALPHA*R/QI)
87 QIB=EXP(BETA*R/QI)
88 QIC=EXP(GAM*R/QI)
89 VI=(A*QIA+B*QIB+C*QIC)/ET
90 GI=R/SQRTF(R**2.-VI*R*QI-RHO(J)**2.*QI**2.)
91 SJA=EXP(ALPHA*R/SJ)
92 SJB=EXP(BETA*R/SJ)
93 SJC=EXP(GAM*R/SJ)
94 VJ=(A*SJA+B*SJB+C*SJC)/ET
95 GJ=R/SQRTF(R**2.-VJ*R*SJ-RHO(J)**2.*SJ**2.)
96 TKA=EXP(ALPHA*R/TK)
97 TKB=EXP(BETA*R/TK)
98 TKC=EXP(GAM*R/TK)
99 VK=(A*TKA+B*TKB+C*TKC)/ET
100 GK=R/SQRTF(R**2.-VK*R*TK-RHO(J)**2.*TK**2.)
101 U=(TK*GI+SJ*GJ+QI*GK)*3.14159/(6.*R)

```

```

102 THETA(J)=THETA(0)+3.14159-2.*RHO(J)*U
103 DGI=R*RHO(J)*QI**2./((SQRTF(R**2.-VI*R*QI-RHO(J)**2.*QI**2.))**3.
104 DGJ=R*RHO(J)*SJ**2./((SQRTF(R**2.-VJ*R*SJ-RHO(J)**2.*SJ**2.))**3.
105 DGK=R*RHO(J)*TK**2./((SQRTF(R**2.-VK*R*TK-RHO(J)**2.*TK**2.))**3.
106 DU=3.14159*(TK*DGI+SJ*DGJ+QI*DGK)/(6.*R)
107 DRDRHO=2.*RHO(J)/(2.*RHO(J)**2./R-R*DV+V)
108 DVI=(A*ALPHA*QIA+B*BETA*QIB+C*GAM*QIC)/ET
109 DVJ=(A*ALPHA*SJA+B*BETA*SJB+C*GAM*SJC)/ET
110 DVK=(A*ALPHA*TKA+B*BETA*TKB+C*GAM*TKC)/ET
111 DGDRJ=(DVI/R-QI*VI/R**2-2.*QI**2*RHO(J)**2/R**3)*(GI**3/2.)
112 DGDRJ=(DVJ/R-SJ*VJ/R**2-2.*SJ**2*RHO(J)**2/R**3)*(GJ**3/2.)
113 DGDRK=(DVK/R-TK*VK/R**2-2.*TK**2*RHO(J)**2/R**3)*(GK**3/2.)
114 DUDR=(TK*DGDRJ+SJ*DGDRJ+QI*DGDRK)*3.14159/(6.*R)-U/R
115 DUDRHO=DUDR*DRDRHO+DU
116 DTHETA=2.*U+2.*RHO(J)*DUDRHO
117 SIGMA=RHO(J)/(SINF(THETA(J))*DTHETA)
118 DRHO=SIGMA*SINF(THETA(J))*SQRTF(8.8/EV(K))/RHO(J)
119 IF(THETA(J)-3.14159)29,30,29
120 DPHI=SQRTF(8.8/EV(K))
121 GO TO 31
122
123 29 DPHI=SQRTF(8.8/EV(K))/SINF(THETA(J))
124 31 DTH=SQRTF(8.8/EV(K))
125 FAC2=1.-COSF(THETA(J)-DTH)
126 FAC1=1.-COSF(THETA(J))
127 DELTA=2.*XMP*XMT/(XMP+XMT)**2
128 PER=100.*(SQRTF(1.-DELTA*FAC2)/(1.-DELTA*FAC1))-1.)
129 ARG=SINF(THETA(J))/((XMP/XMT)+COSF(THETA(J)))
130 IF(ARG)41,41,42
131 41 ARG=1000000.
132 42 THETA(J)=ATANF(ARG)
133 204 DEG(J)=THETA(J)*180./3.14159
134 125 RAD=1./529
135 P=RHO(J)*DRHO*DPHI/(3.14159*RAD**2.)
136 IF(P-1.)9,9,8
137 8 P=1.
138 9 GS=SIGMA*P

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139*
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      IF(CS)12,12,11
11  CSL(J)=LOGF(CS)
      IF(DEG(J)-90.)13,6,6
13  IF(DEG(J)-2.)6,6,12
12  PRINT5,EV(K),RHO(J),R,DEG(J),SIGMA,P,CS,PER
      5  FORMAT(F8.2,2F12.3,F9.2,1P3E13.3,F15.2)
      6  CONTINUE
120  CALL DRAW(101,DEG(J),CSL(J),NOA,0,LABEL(K),ITITLE,10.,0,0,0,0,0,
      19,15,1,LAST)
15  GOTO138
      7  END
      END
      * STATEMENT INDEX 138  EP=EV(K)/2.

```

EXPLANATION OF PROGRAM

STATEMENT INDEX

1-5	Places and prints column headings for print out.
6-8	Dimension statements. Self explanatory.
9-23	Do loop for graph title.
24-29	Constants for the potential used. See equation No. 6, Appendix 1. May take on any values in accordance with potential used.
30	Sets the initial value for the number of iterations. See statement index 74 and 75.
31	Sets the initial value of the impact parameter such that $RH0(1) = 0$. See statement index 60
32	Sets the initial value of theta, the scattering angle in C. M. Coordinates.
33	Sets the initial value of the energy of the hydrogen molecular ion in the LAB. Coordinate system, EV, such that $EV(1) = 1000\text{ev}$. See statement index 37.
34, 39, 40, 41, 42, 43, 44, 45	Give the draw program the proper parameter to draw 10 curves on one graph.
35	Begins outer do loop for 10 different energies defined by statement index 33 and 37.
36	Subscript relationship to achieve desired energies.
37	Energy defining relationship. May be varied for desired energies.
38	Sets the initial value of R for the iteration to find the root of equation 4, Appendix 2. May be based on b, the collision diameter. (Page 19)
47-57	Label program for the labeling of curves with appropriate energy.
58	Begins inner do loop for 101 values of the impact parameter, RH0, as defined by statement index 31 and 60. RH0 is in units of a_0
59	Subscript relationship to achieve desired values of RH0.

60	Defining relationship for $RH0$. May be varied as desired.
61-63	Evaluates the exponential terms of the potential used.
64	Mass of the projectile particle in a. m. u.
65	Mass of the target particle in a. m. u.
66	Evaluates the relative energy factor of equation 4, Appendix 1 in terms of EV.
67	Evaluates V as defined by equation 8, Appendix 1.
68	Evaluates equation 11, Appendix 1, for the iteration.
69	Evaluates DV as defined by equation 13, Appendix 1, for the iteration.
70	Evaluates equation 12, Appendix 1.
71	Computes a new value of R for the iteration.
72-73	Compares the last two values of R.
74	Counts the number of iterations.
75	Stops the program if finding R requires over 10000 iterations.
76	Replaces R with the last value computed by statement index 71.
77	Repeats the iteration if statement index 73 has not been satisfied.
78	Continues the program if statement index 73 has been satisfied.
79-81	Insures that the proper value of R has been used to compute V and DV.
82	Stops the program if R is less than $RH0$ and exits the inner do loop if $R = RH0$.
83-85	Evaluate the cosine functions of equation 15, Appendix 1.
86-100	Evaluate the $g(X_1)$ as defined by equation 16, Appendix 1.

101 Evaluates the integral U as defined by equation 15, Appendix 1.

102 Computes theta the scattering angle in the C. M. coordinate system for the given energy and impact parameter by equation 2, Appendix 1.

103-105 Computes the $\partial g(x)/\partial \rho$ as defined by equation 21, Appendix 1.

106 Evaluates $\partial U/\partial \rho$ as defined by equation 20, Appendix 1.

107 Computes $dR_0/d\rho$ as defined by equation 22, Appendix 1.

108-113 Computes the $\partial g(x)/\partial R_0$ as defined by equations 24, Appendix 1.

114 Computes $\partial U/\partial R_0$ as defined by equation 23 Appendix 1.

115 Computes $dU/d\rho$ as defined by equation 19, Appendix 1.

116 Computes $|d\theta/d\rho|$ as defined by equation 18, Appendix 1.

117 Computes the differential cross section for scattering of protons at the previously computed angle by equation 1, Appendix 1.

118 Computes $\Delta \rho$ as given on page 16.

119 Prevents dividing by zero in statement index 122 when theta is 180.

120 A dummy statement to give a value of $\Delta \Phi$ for theta = 180.

121 Skips statement index 122 when theta = 180°.

122 Evaluates $\frac{\Delta \Phi}{\sqrt{2}}$ as given on page 16.

123 Evaluates $\frac{\Delta \theta}{\sqrt{2}}$ as given on page 16.

124-127 Compute the percent difference in velocities after scattering as described on page 24.

128-132 Convert the scattering angle, theta, to LAB coordinates and degrees.

- 133 Gives the inter atomic spacing ℓ .
- 134 Computes the value of the orientation probability as defined on page
- 135-136 Limits the value of P to 1.
- 137 Computes the differential cross section for H_2^+ scattering as given on page 13.
- 138 Gives the proton energy for printing when that is of interest.
- 139 Prevents the log. function from having a negative or zero argument in statement index 140.
- 140 Computes the logarithm of the crosssection for the draw program.
- 141-142 Limits the values of the scattering angle printed to those between 2° and 90° .
- 143 Prints results for each value of RHO assigned.
- 144-150 Self explanatory.

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13. ABSTRACT

The primary problem in the calculation of the differential scattering cross section for hydrogen molecular ions is the derivation of an approximate expression for the probability that the hydrogen molecular ion will be oriented, prior to impact, in such a way as to avoid disruption during scattering. Using a simple model, an approximate expression for the orientation probability is obtained. Differential cross sections for the scattering of hydrogen molecular ions from carbon and krypton are calculated using classical scattering theory and the derived orientation probability. Impact energies of 100 to 1000 electron volts are considered. In addition differential cross sections for protons scattered from carbon and krypton are presented.

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KEY WORDS

LINK A

LINK B

LINK C

ROLE

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Scattering Cross Section

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